

IUCLID

DATA SET

Existing Chemical **Benzene, C6-12 Alkyl Derivatives (CAS# 68608-80-0)**

Producer
Company: **Huntsman Corporation**
Creation date: **May 2, 2001**

Prepared by
Company: **THE WEINBERG GROUP INC.**

Printing date: **November 8, 2001**
Revision date:
Date of last update: **November 8, 2001**

Number of pages: **44**

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I U C L I D

Data Set

Existing Chemical Substance ID: Atops

Producer Related Part

Company: The Weinberg Group Inc.
Creation date: 02-MAY-2001

Substance Related Part

Company: The Weinberg Group Inc.
Creation date: 02-MAY-2001

Printing date: 08-NOV-2001

Revision date:

Date of last Update: 08-NOV-2001

Number of Pages: 44

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7

Reliability (profile): Reliability: without reliability, 1, 2, 3, 4

Flags (profile): Flags: without flag, confidential, non confidential, WGK
(DE), TA-Luft (DE), Material Safety Dataset, Risk
Assessment, Directive 67/548/EEC

1.0.1 OECD and Company Information**Name:** Huntsman Corporation

03-OCT-2001

1.0.2 Location of Production Site**Remark:** The production site is located in North America.

03-OCT-2001

1.0.3 Identity of Recipients**Remark:** Not applicable

03-OCT-2001

1.1 General Substance Information**Substance type:** organic**Physical status:** liquid**Remark:** Alkylate benzene mixture derived as a lower boiling point co-product from the LAB manufacturing process. Benzene, C6-12 alkyl derivs. (68608-80-0)

05-NOV-2001

1.1.1 Spectra**Remark:** Not applicable

03-OCT-2001

1.2 Synonyms**Remark:** Alkylate Top

22-OCT-2001

1.3 Impurities**CAS-No:****EINECS-No:****EINECS-Name:****Remark:** Not specified

03-OCT-2001

1.4 Additives**CAS-No:****EINECS-No:****EINECS-Name:****Remark:** Not specified
03-OCT-2001**1.5 Quantity****Quantity** 1 000 - 5 000 tonnes
08-NOV-2001**1.6.1 Labelling****Labelling:****Remark:** There are no specific labeling requirements for the alkylate top.
03-OCT-2001**1.6.2 Classification****Classification:****Class of danger:****R-Phrases:****Remark:** There are no specific classification requirements for the alkylate top.
03-OCT-2001**1.7 Use Pattern****Type:****Category:****Remark:** Greater than 95% of the alkylate top is used as auxiliary fuel.
03-OCT-2001**1.7.1 Technology Production/Use****Remark:** Not applicable
03-OCT-2001**1.8 Occupational Exposure Limit Values****Type of limit:****Limit value:****Remark:** No TLV's have been established.
03-OCT-2001

1.9 Source of Exposure

Memo: Very limited potential for human or environmental exposure.
03-OCT-2001

1.10.1 Recommendations/Precautionary Measures

Remark: Use of appropriate personel protective equipment.
03-OCT-2001

1.10.2 Emergency Measures

Remark: Flush with water. Ventilate area. Wipe up or absorb on
suitable material and shovel into appropriate container.
03-OCT-2001

1.11 Packaging

Memo: Product is available in tank cars and tank trucks.
03-OCT-2001

1.12 Possib. of Rendering Subst. Harmless

**Type of
destruction:**

Remark: Flush with water
03-OCT-2001

1.13 Statements Concerning Waste

Memo: Dispose of waste in accordance with appropriate RCRA and local
requirements.
03-OCT-2001

1.14.1 Water Pollution

Classified by:
Labelled by:
Class of danger:
Remark: Not required
03-OCT-2001

1.14.2 Major Accident Hazards

Legislation:

Substance listed:

Remark: As with all chemicals, avoid contact with skin, eyes or clothing.

03-OCT-2001

1.14.3 Air Pollution

Classified by:

Labelled by:

Number:

Class of danger:

Remark: Not required

03-OCT-2001

1.15 Additional Remarks

Memo: None

03-OCT-2001

1.16 Last Literature Search

Date of Search: 15-AUG-2001

03-OCT-2001

1.17 Reviews

Memo: None

03-OCT-2001

1.18 Listings e.g. Chemical Inventories

Additional Info: Listed on TSCA Inventory, Canadian DSL, and EINECS or ELINCS

03-OCT-2001

2.1 Melting Point

Value: < -70 degree C
Decomposition: no
Sublimation: no
Method: other: DIN 51 583
GLP: no data
Remark: No data specifying done as GLP, but presumed GLP based on reported use of DIN protocol.
Source: Wibarco 1993.
Test substance: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Reliability: (2) valid with restrictions
Reported in LAB Risk Assessment document citing a DIN protocol.

25-JUL-2001

(7)

Value: = 10 degree C
Method: other: no data
GLP: no data
Test substance: Pentadecane (C15 normal paraffin) (629-62-9)
Reliability: (2) valid with restrictions
Standard reference text.

22-OCT-2001

Value: = 6 degree C
Method: other: no data
GLP: no data
Source: Dean 1979.
Test substance: Tetradecane (C14 normal paraffin) (629-59-4)
Reliability: (2) valid with restrictions
Standard reference text.

02-NOV-2001

(11)

Value: = -14 degree C
GLP: no data
Source: Jeng 1992.
Test substance: Decylbenzene (104-72-3)
Reliability: (1) valid without restriction

25-JUL-2001

(26)

Value: = -24 degree C
GLP: no data
Source: Jeng 1992.
Test substance: Nonylbenzene (1081-77-2)
Reliability: (1) valid without restriction

25-JUL-2001

(26)

2.2 Boiling Point

Value: = 278 - 314 degree C at 1013 hPa
Decomposition: yes
Method: other: ASTM D 86
Year: 1989
GLP: no
Source: EniChem Augusta Industriale 1993.
Test substance: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Reliability: (2) valid with restrictions
Reported in LAB Risk Assessment document.
25-JUL-2001 (13)

Value: = 240 - 250 degree C
GLP: no data
Source: Huntsman MSDS 2000.
Test substance: Alkylate L-210 (Benzene, C6-12 alkyl derivatives; 68608-80-0)
Reliability: (4) not assignable
Data from MSDS but original study report not available for review.
25-JUL-2001 (22)

Value: = 271 degree C
Method: other: no data
GLP: no data
Source: Dean 1979.
Test substance: Pentadecane (C15 normal paraffin) (629-62-9)
Reliability: (2) valid with restrictions
Standard reference text.
01-NOV-2001 (11)

Value: = 253 degree C
Method: other: no data
GLP: no data
Source: Dean 1979.
Test substance: Tetradecane (C14 normal paraffin) (629-59-4)
Reliability: (2) valid with restrictions
Standard reference text.
01-NOV-2001 (11)

Value: = 276 - 286 degree C
Method: other: Internal laboratory analysis
GLP: no data
Remark: Normal boiling points at 1 atm for 2, 3, 4, and 5-phenyldodecanes.
Source: Huntsman 2001.
Test substance: C10-LAB
Reliability: (2) valid with restrictions
05-NOV-2001 (23)

Value: = 262 - 286 degree C
GLP: no
Method: Estimation of C9-LAB 2, 3, 4, and 5 phenyl isomers based on a regression analysis of the C10-C14 LAB positional isomer data.
Source: Rapko 2001.
Test substance: C9-LAB
Reliability: (2) valid with restrictions
08-NOV-2001 (34)

Value: = 300 degree C
Method: other: no data
GLP: no data
Source: Dean 1979.
Test substance: Decylbenzene (104-72-3)
Reliability: (2) valid with restrictions
Standard reference text.
01-NOV-2001 (11)

Value: = 282 degree C
Method: other: no data
GLP: no data
Source: Dean 1979.
Test substance: Nonylbenzene (1081-77-2)
Reliability: (2) valid with restrictions
Standard reference text.
01-NOV-2001 (11)

2.3 Density

Type:
Value:
Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

2.3.1 Granulometry

**Type of
distribution:**

Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

2.4 Vapour Pressure

Value: = .0017 hPa at 25 degree C
Method: other (calculated)
GLP: no
Source: EPIWIN V.3.10
Test substance: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Reliability: (2) valid with restrictions
Standard EPA peer-reviewed database and estimation software.
25-JUL-2001

Value: = .0046 hPa at 25 degree C
GLP: no data
Source: Daubert 1989.
Test substance: Pentadecane (C15 normal paraffin) (629-62-9)
Reliability: (2) valid with restrictions
Cited in HSDB but original report not available for review.
25-JUL-2001 (42)

Value: = .0155 hPa at 25 degree C
GLP: no data
Source: Daubert 1989.
Test substance: Tetradecane (C14 normal paraffin) (629-59-4)
Reliability: (2) valid with restrictions
Cited in HSDB but original report not available for review.
02-NOV-2001 (10)

Value: = .0017 hPa at 25 degree C
GLP: no data
Source: Daubert 1989.
Test substance: Decylbenzene (104-72-3)
Reliability: (2) valid with restrictions
Cited in HSDB but original report not available for review.
02-NOV-2001 (10)

Value: = .0076 hPa at 25 degree C
Method: other (calculated)
GLP: no data
Source: EPIWIN V.3.10
Test substance: Nonylbenzene (1081-77-2)
Reliability: (2) valid with restrictions
Standard EPA peer-reviewed database and estimation software.
02-NOV-2001 (46)

2.5 Partition Coefficient

log Pow: = 7.5 - 9.12 at 25 degree C
Method: other (calculated): Fragment constants by Hansch and Leo
Year: 1979
GLP: no
Remark: The individual calculated values using the fragment constant method are 7.5, 8.04, 8.58, and 9.12 for LABs of alkyl chain length C10, C11, C12, and C13, respectively.
Source: Sherblom et al 1988; Hansch and Leo.
Test substance: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Reliability: (2) valid with restrictions
25-JUL-2001 (17) (41)

log Pow: = 7.72
Method: other (calculated): Extrapolated from Hutchinson et al
Year:
GLP: no data
Source: Coates et al 1985; Hutchinson et al 1980.
Test substance: Pentadecane (C15 normal paraffin) (629-62-9)
Reliability: (2) valid with restrictions
25-JUL-2001 (8) (24)

log Pow: = 7.2
Method: other (measured): Head space chromatographic method
Year:
GLP: no data
Source: Sangster 1989; Coates et al 1985.
Test substance: Tetradecane (C14 normal paraffin) (629-59-4)
Reliability: (1) valid without restriction
25-JUL-2001 (8) (40)

log Pow: = 7.35
Method: other (measured): Shake flask
Year:
GLP: no data
Source: Sangster 1989; Bruggeman et al 1982.
Test substance: Decylbenzene (104-72-3)
Reliability: (1) valid without restriction
01-NOV-2001 (5) (40)

log Pow: = 7.11
Method: other (calculated): EPIWIN V.3.10
Year:
GLP: no data
Test substance: Nonylbenzene (1081-77-2)
Reliability: (2) valid with restrictions
Standard EPA peer-reviewed database and estimation software.
25-JUL-2001

2.6.1 Water Solubility

Value: = .041 mg/l at 27 degree C
Qualitative: of very low solubility
Method: other: Monsanto method
GLP: yes
Remark: Gas chromatographical determination: aqueous solubility was reported as the sum of linear C9-13 alkylbenzene GC peak areas.
Source: Gledhill et al 1991.
Test substance: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Reliability: (1) valid without restriction
25-JUL-2001 (16)

Value: = .037 mg/l
GLP: yes
Method: Six mL of LAB were deposited on the top of approximately 700 mL of ultra-pure water in a reaction vessel. The solution was stirred and maintained at 20-23 degrees Celcius. After 96 hours, 100 mL aliquots were sampled and the water accommodated fraction determined.
Remark: The WAF were determined to be 0.037, 0.040, and 0.049 mg/L for LAB, Phenyl C-10, and Phenyl C-12, respectively. The total solubility seems to be independent of the number of components in the mixture, and therefore for a single compound, the final water concentration in saturated solutions will depend on the total number of isomers/homologues present in the mixture. Further, the relative composition of the saturated solutions differs from that observed for the mixture, these differences

seem to be regulated by a more complex mechanism than liphophilicity.

Source: Alonso et al 1999.
Test substance: Phenyl-C10 (C10 LAB) and LAB (67774-74-7)
Reliability: (1) valid without restriction
03-OCT-2001 (2)

Value: < 1000 mg/l
GLP: no data
Remark: Data listed in MSDS as < 0.1%.
Source: Huntsman 2000.
Test substance: Alkylate L-210 (Benzene, C6-12 alkyl derivatives; 68608-80-0)
Reliability: (4) not assignable
Data from MSDS but original study report not available for review.
03-OCT-2001 (22)

Value: = .00008 mg/l
Method: other: Extrapolated from Hutchinson et al
GLP: no data
Source: Coates et al 1985; Hutchinson et al 1980.
Test substance: Pentadecane (C15 normal paraffin) (629-62-9)
Reliability: (2) valid with restrictions
25-JUL-2001 (8) (24)

Value: = .0022 mg/l at 25 degree C
Method: other: Shake flask
Remark: Methods meeting current standards were used. Flasks were shaken gently for 12-hours, then allowed to sit at 25 plus or minus 0.1 degrees Celcius for another 24 hours to allow dispersed droplets to rise to the surface. Aliquots of 100 mL were removed and filtered through a 0.45 micrometer Millipore filter to remove any small hydrocarbon droplets still in suspension. This filtration step is necessary to remove colloidal hydrocarbon and to determine a true water solubility.
Source: Sutton and Calder 1974.
Test substance: Tetradecane (C14 normal paraffin) (629-59-4)
Reliability: (1) valid without restriction
25-JUL-2001 (43)

Value: = .0024 mg/l
GLP: no data
Source: Krop et al 1997.
Test substance: Decylbenzene (104-72-3)
Reliability: (2) valid with restrictions
As cited in HSDB.
25-JUL-2001 (27)

Value: = .035 mg/l at 25 degree C
Method: other: EPIWIN V.3.10
GLP: no data
Test substance: Nonylbenzene (1081-77-2)
Reliability: (2) valid with restrictions
Standard EPA peer-reviewed database and estimation software.
25-JUL-2001

2.6.2 Surface Tension

Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

2.7 Flash Point

Value: ca. 117 degree C
Type:
Method:
Year:
Source: Huntsman Petrochemical Corporation 2000.
Test substance: Alkylate L-210 (Benzene, C6-12 alkyl derivatives; 68608-80-1)
22-OCT-2001 (22)

2.8 Auto Flammability

Value:
Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

2.9 Flammability

Result:
Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

2.10 Explosive Properties

Result:
Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

2.11 Oxidizing Properties

Result:
Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

2.12 Additional Remarks

Memo: None
01-NOV-2001

3.1.1 Photodegradation

Type: other: Acetonitrite solution
Light source: Sun light
Rel. intensity: = 1 based on Intensity of Sunlight
Conc. of subst.: 2 mg/l at 18 degree C
DIRECT PHOTOLYSIS
Degradation: < 1 % after 14 day
Method: other (measured): EPA
Year: 1979 **GLP:** no
Test substance: other TS: Alkylate 215 (LAB) (67774-74-7)
Method: Test solutions were exposed to natural sunlight for 14 days during the summer (52% possible sunlight). Controls wrapped in aluminum foil were also included. Duplicate photolysis tubes were sacrificed at 0, 2, 5, 9, and 14 days and analyzed by HPLC.
Remark: Greater than 99% of the original material remained at the end of the test period. As natural water solutions were not used, sensitized photolysis tubes were sacrificed at 0, 2, 5, 9, and 14 days and analyzed by HPLC.
Source: Gledhill 1991.
Reliability: (1) valid without restriction
22-OCT-2001 (16)

Type:
DIRECT PHOTOLYSIS
Halflife t1/2: = 7.1 hour(s)
Method: other (calculated): EPIWIN V.3.10
Year: **GLP:** no
Test substance: other TS: Pentadecane (C15 normal paraffin) (629-62-9)
Remark: Hydroxyl radical reaction in air calculated from its estimated rate constant of 1.82×10^{-11} cm cubed/mol-sec at 25 degrees Celcius determined using the structure estimation method of Meylan and Howard.
Source: USEPA and Syracuse Research Corporation 2000.
Reliability: (2) valid with restrictions
Standard EPA peer-reviewed database and estimation software.
22-OCT-2001 (46)

Type:
DIRECT PHOTOLYSIS
Halflife t1/2: = 7.7 hour(s)
Method: other (calculated): EPIWIN V.3.10
Year: **GLP:** no
Test substance: other TS: Tetradecane (C14 normal paraffin) (629-59-4)
Remark: Hydroxyl radical reaction in air calculated from its estimated rate constant of 1.68×10^{-11} cm cubed/mol-sec at 25 degrees Celcius determined using the structure estimation method of Meylan and Howard.
Source: USEPA and Syracuse Research Corporation 2000.
Reliability: (2) valid with restrictions
Standard EPA peer-reviewed database and estimation software.
22-OCT-2001 (46)

Type:**DIRECT PHOTOLYSIS****Halflife t1/2:** = 7.5 hour(s)**Method:** other (calculated): EPIWIN V.3.10**Year:** **GLP:** no**Test substance:** other TS: Decylbenzene (104-72-3)**Remark:** Hydroxyl radical reaction in air calculated from its estimated rate constant of 1.72×10^{-11} cm cubed/mol-sec at 25 degrees Celcius determined using the structure estimation method of Meylan and Howard.**Source:** USEPA and Syracuse Research Corporation 2000.**Reliability:** (2) valid with restrictions
Standard EPA peer-reviewed database and estimation software.

22-OCT-2001

(46)

Type:**DIRECT PHOTOLYSIS****Halflife t1/2:** = 8.1 hour(s)**Method:** other (calculated): EPIWIN V.3.10**Year:** **GLP:****Test substance:** other TS: Nonylbenzene (1081-77-2)**Remark:** Hydroxyl radical reaction in air calculated from its estimated rate constant of 1.58×10^{-11} cm cubed/mol-sec at 25 degrees Celcius determined using the structure estimation method of Meylan and Howard.**Source:** USEPA and Syracuse Research Corporation 2000.**Reliability:** (2) valid with restrictions
Standard EPA peer-reviewed database and estimation software.

22-OCT-2001

(46)

3.1.2 Stability in Water**Type:****Method:****Year:** **GLP:****Test substance:** other TS: Benzene, C6-12 alkyl derivatives (68608-80-0)**Remark:** Stable. Hydrolysis is not expected to occur due to the lack of hydrolyzable functional groups.

03-OCT-2001

3.1.3 Stability in Soil**Type:****Radiolabel:****Concentration:****Cation exch.**

capac.

Microbial

biomass:

Method:**Year:** **GLP:****Test substance:****Remark:** Not a High Production Volume Challenge Program endpoint.

03-OCT-2001

3.2 Monitoring Data (Environment)

Type of
measurement:

Medium:

Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

3.3.1 Transport between Environmental Compartments

Type:

Media:

Method:

Year:

Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

3.3.2 Distribution

Media:

Method:

Year:

Remark: Not applicable
03-OCT-2001

3.4 Mode of Degradation in Actual Use

Memo: Biodegradation
03-OCT-2001

3.5 Biodegradation

Type: aerobic

Inoculum: domestic sewage, adapted

Concentration: 20 mg/l related to DOC (Dissolved Organic Carbon)

Degradation: = 67 % after 28 day

Result: readily biodegradable

Kinetic:

7 day	= 0 %
10 day	= 14 %
14 day	= 30 %
25 day	= 65 %
28 day	= 67 %

Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"

Year: GLP: yes

Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)

Remark: The biodegradation was measured by CO2 evolution. An emulgator was added to disperse the poorly soluble LAB.

Source: Huls 1987.

Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.

25-JUL-2001

(18)

Type: aerobic
Inoculum: domestic sewage
Contact time: 28 day
Degradation: = 64 % after 28 day
Result: readily biodegradable
Method: OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"

Year: **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Source: Istituto Guido Donegani 1995.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.

03-OCT-2001

(25)

Type: aerobic
Inoculum: other: not specified
Concentration: 18 mg/l related to Test substance
Contact time: 35 day
Degradation: = 56 - 61 % after 35 day
Method: other: Shake Flask Carbon Evolution Procedure
Year: 1975 **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Remark: The degradation was less than in other studies, possibly because the test was conducted at LAB concentrations far exceeding the solubility limit. For this reason, studies in more natural systems (Standard River Die-away Test) were carried out using lower LAB concentrations (100-500 ppb) and GC analytical determination. The results show a primary biodegradation of > 90% and a half-life of 4-15 days. Sewage treatment plants remove most of LAB released in sewage. Average percent removals from > 69% to > 98% for trickling filter and activated sludge plants, respectively, are reported.

Source: Gledhill et al 1991.
Reliability: (1) valid without restriction

25-JUL-2001

(16)

Type: aerobic
Inoculum: other: Soil, raw sewage, and activated sludge mixed liquor
Degradation: = 46 % after 35 day
Method: other: Monsanto shake flask procedure
Year: **GLP:** no data
Test substance: other TS: L-210L (Benzene, C6-12 alkyl derivatives; 68608-80-0)
Method: An acclimated inoculum is prepared by the stepwise addition of test compound to a defined medium over a 14-day period. After acclimation, 100 mL of inoculum are mixed with 900 mL of minimal salts media. After aerating the mixture with 70% oxygen in nitrogen, a known quantity of test component is added to each flask. An open reservoir containing 10 mL of 0.15N barium hydroxide is suspended via a glass tube inserted in a neoprene stopper. After sealing, the flasks are agitated in the dark at ambient temperature. Periodic removal and titration of the barium hydroxide solution are used to determine the CO₂ evolved. CO₂ evolution values obtained with the control are subtracted from values for the test compound.
Remark: The light aromatic naphtha (L-210L) is predominantly a mixture of paraffins, alkylbenzene, and indanes. The CO₂ evolution of 46% of theory probably arises from degradation of the paraffin and alkylbenzene components. The L-210L tested (in 1980) consisted of 29% paraffin, 44% alkylbenzene, 24% indanes, with an avg.C # = 13.5. Because of advances in the production process, the current composition is approximately 40% paraffins and 60% alkylbenzenes. Therefore, this study likely under predicts the actual biodegradation of the current product.
Source: Saeger 1980.
Reliability: (1) valid without restriction
25-JUL-2001 (29) (38)

Type: aerobic
Inoculum: other: Enriched sediment medium
Degradation: = 75 % after 8 day
Method: other: Experimental conditions have been devised to accelerate the processes of degradation of hydrocarbons in sediments.
Year: **GLP:** no data
Test substance: other TS: Pentadecane (C15 normal paraffin) (629-62-9)
Method: Sediments previously freed from all organic matter were used. After drying, these sediments were mixed with pentadecane. The material was then incubated for 8 days in a medium containing an initial bacterial MLP inoculum of 1x10E+8 cells/g of sediment. At the end of the incubation period the sediment was harvested and extracted. The FA fraction was analyzed.
Remark: The experimental conditions make it possible to determine the correlations between bacterial activity and the accumulation of petroleum constituents and so lead to a better knowledge of the potentialities of auto-purification of the marine medium.
Source: Azoulay et al 1983.
Reliability: (2) valid with restrictions
02-NOV-2001 (3)

Type: aerobic
Inoculum:
Degradation: 100 % after 56 day
Method:
Year: **GLP:**
Test substance: other TS: Pentadecane (C15 normal paraffin) (629-62-9)
Method: Heated crude oil was added to a concentration of 1 g/L to a natural seawater medium. This solution was cultivated at 20 degrees Celcius under constant shaking (100 strokes/min) to promote the growth of indigenous oil-degrading microorganisms. The abundance of approximately 50 constituent compounds was determined using GC-MS in SIM mode after 8 weeks.
Remark: Pentadecane was 100% biodegraded within 8 weeks.
Source: Dutta and Harayama 2000.
Reliability: (1) valid without restriction
25-JUL-2001 (12)

Type: aerobic
Inoculum:
Degradation: 100 % after 56 day
Method:
Year: **GLP:**
Test substance: other TS: Tetradecane (C14 normal paraffin) (629-59-4)
Method: Heated crude oil was added to a concentration of 1 g/L to a natural seawater medium. This solution was cultivated at 20 degrees Celcius under constant shaking (100 strokes/min) to promote the growth of indigenous oil-degrading microorganisms. The abundance of approximately 50 constituent compounds was determined using GC-MS in SIM mode after 8 weeks.
Remark: Tetradecane was 100% biodegraded within 8 weeks.
Source: Dutta and Harayama 2000.
Reliability: (1) valid without restriction
25-JUL-2001 (12)

Type:
Inoculum:
Result: other: Biodegrades easily
Method: other: No data
Year: **GLP:** no data
Test substance: other TS: Tetradecane (C14 normal paraffins) (629-59-4)
Remark: Tetradecane was listed as a compound that biodegrades and was classified in level 2 (degraded without much difficulty) in a 5-tiered rating system on ease of biodegradability.
Source: Abrams et al 1975.
Reliability: (2) valid with restrictions
As cited in HSDB.
25-JUL-2001 (1)

Type: aerobic
Inoculum: other: Enriched sediment medium
Degradation: = 72 % after 8 day
Method: other: Experimental conditions have been devised to accelerate the processes of degradation of hydrocarbons in sediments.
Year: **GLP:** no data
Test substance: other TS: Nonylbenzene (1081-77-2)
Method: Sediments previously freed from all organic matter were used. After drying, these sediments were mixed with nonylbenzene. The material was then incubated for 8 days in a medium containing an initial bacterial MLP inoculum of 1x10E+8 cells/g of sediment. At the end of the incubation period the sediment was harvested and extracted. The FA fraction was analysed.
Remark: The experimental conditions make it possible to determine the correlations between bacterial activity and the accumulation of petroleum constituents and so lead to a better knowledge of the potentialities of auto-purification of the marine medium.
Source: Azoulay et al 1983.
Reliability: (2) valid with restrictions
03-OCT-2001 (3)

Type: aerobic
Inoculum: other: Alcaligenes sp. PHY12 originating from a mixed bacterial community isolated from seafoam
Degradation: = 65 % after 10 day
Method:
Year: **GLP:** no data
Test substance: other TS: Nonylbenzene (1081-77-2)
Method: Pyrex flasks containing 120 mL of medium composed of seawater supplemented with yeast extract, ammonium chloride, sodium phosphate and n-nonylbenzene were used. Aeration was realized with strong agitation at 30 degrees Celcius on a reciprocal shaker (96 rpm). Traces of anthraquinone were added as a photosensitivity agent.
Remark: The reported degradation value is for biodegradation alone. Concurrent studies demonstrate that in the presence of light, photo-oxidation of the more refractory biodegradation products results in even greater total degradation (84% in 10 days).
Source: Rotani 1987.
Reliability: (1) valid without restriction
22-OCT-2001 (37)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: Not a High Production Volume Challenge Program endpoint.
01-NOV-2001

3.7 Bioaccumulation

Species:

Exposure period:

Concentration:

BCF:

Elimination:

Method:

Year:

GLP:

Test substance:

Remark: Not a High Production Volume Challenge Program endpoint.
01-NOV-2001

3.8 Additional Remarks

Memo: None

01-NOV-2001

AQUATIC ORGANISMS**4.1 Acute/Prolonged Toxicity to Fish**

Type: other: Static daily renewal
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 14 day
Unit: mg/l **Analytical monitoring:** yes
LC50: > .0055
Method: other: OECD Guideline 202
Year: 1984 **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Method: The LAB tested was comprised of 93% alkylbenzenes and 18% phenylalkanes. The relative percentage of the C10-13 homologues is 14:34:31:21, respectively. The treatment solutions were prepared by adding 5 g of LAB to 5 L of reconstituted water. After being vigorously stirred for 24 hours and allowed to stand for 4 hours, the aqueous phase was separated and filtered. This solution was the solubility concentration and was used in the experiment. In addition to the undiluted concentration, two more test concentrations were obtained by 2:1 and 1:1 dilutions with reconstituted water. Test solutions were renewed daily.
Remark: No toxic effects were observed. Measured concentrations in the undiluted sample at the beginning of the study ranged from 0.0046 to 0.0065 mg/L (mean=0.0055).
Source: Calcinai et al 2001.
Reliability: (1) valid without restriction
03-OCT-2001 (6)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: > 1000
Method: other: EPA-660/3-7-009: Method for acute toxicity tests with fish, macroinvertebrates and amphibians.
Year: 1975 **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Remark: The test shows no adverse effects after 96 hours at nominal concentration (1000 mg/L) up to and exceeding the water solubility using a solvent carrier. Rainbow trout and fathead minnows were also tested with the same results.
Source: Gledhill et al 1991.
Reliability: (1) valid without restriction
03-OCT-2001 (16)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC50: > 1000
Method: other: Bestimmung der Wirkung von wasserinhaltsstoffen auf Fische, DIN 38412 Teil 15
Year: 1982 **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Remark: This test shows no adverse effects after 48 hours at nominal concentration (1000 mg/L) up to and exceeding the water solubility using an emulsifier.
Source: Huls 1994.
Reliability: (2) valid with restrictions
Reported in LAB Risk Assessment document.

25-JUL-2001

(19)

Type: flow through
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 21 day
Unit: mg/l **Analytical monitoring:** yes
LC50: > .079
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1992 **GLP:** yes
Test substance: other TS: Phenyl-C10 (C10 LAB) and LAB (67774-74-7)
Remark: Fish were exposed to duplicate chambers of a single concentration (limit test) in a flow through system. Acetone was used as a solvent. The mean measured concentrations were 0.058 and 0.079 mg/L for the LAB and phenyl C-10, respectively. These assayed concentrations were higher than water solubility limits.
The exposure period lasted up to 3 weeks.
Result: No toxic effects were observed.
Source: Fernandez et al 2000.
Reliability: (1) valid without restriction

03-OCT-2001

(14)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: > 1000
Method: other: Methods of acute toxicity tests with fish, macroinvertebrates, and amphibians
Year: 1975 **GLP:** yes
Test substance: other TS: L210-L (Benzene, C6-12 alkyl derivs.; CAS # 68608-80-0)
Remark: No adverse effects were observed after 96 hours at nominal concentrations up to 1000 mg/L. Acetone was used as a solvent to enhance solubility.
Source: Thompson and Griffen 1981.
Reliability: (2) valid with restrictions

25-JUL-2001

(44)

Type: flow through
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 7 day
Unit: mg/l **Analytical monitoring:** yes
NOEC: > 1240
Method:
Year: 1983 **GLP:** yes
Test substance: other TS: Tetradecane (C14 normal paraffin) (629-59-4)
Method: Rainbow trout were fed experimental diets containing a mixture of n-paraffins. Fish were fed twice a day (at 0900 h and 1630 h) for seven days. Feces were recovered automatically and the relative absorption of different carbon chain lengths was measured. All fish were maintained at 14 degrees Celcius in a 50 liter aquaria under a constant flow of 4 L/min and a 12 hour photoperiod.
Remark: No mortality was observed in the study.
Source: Cravedi 1983.
Reliability: (1) valid without restriction
03-OCT-2001 (9)

Type: flow through
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 7 day
Unit: mg/l **Analytical monitoring:** yes
NOEC: > 2110
Method:
Year: 1983 **GLP:** yes
Test substance: other TS: Pentadecane (C15 normal paraffin) (629-62-9)
Method: Rainbow trout were fed experimental diets containing a mixture of n-paraffins. Fish were fed twice a day (at 0900 h and 1630 h) for seven days. Feces were recovered automatically and the relative absorption of different carbon chain lengths was measured. All fish were maintained at 14 degrees Celcius in a 50 liter aquaria under a constant flow of 4 L/min and a 12 hour photoperiod.
Remark: No mortality was observed in the study. The maximum digestibility of all n-paraffins tested was observed for pentadecane.
Source: Cravedi 1983.
Reliability: (1) valid without restriction
02-NOV-2001 (9)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
NOEC: > .013
EC50: > .013
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: **GLP:** yes
Test substance: other TS: A commercial LAB produced in an HF alkylation process (67774-74-7)
Method: The LAB tested was comprised of 93% alkylbenzenes and 18% phenylalkanes. The relative percentage of the C10-C13 homologues is 14:34:31:21, respectively. The treatment solutions were prepared by adding 5 g of LAB to 5 L of reconstituted water. After being vigorously stirred for 24 hours and allowed to stand for 4 hours, the aqueous phase was separated and filtered. This solution was the solubility concentration and was used in the experiment. Measured concentrations at the end of the 48-hour study were 0.010 to 0.013 mg/L.
Remark: No effects of immobilization were observed at the solubility concentration.
Source: Calcinai et al 2001.
Reliability: (1) valid without restriction
03-OCT-2001 (6) (47)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: > .04
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: other TS: A commercial LAB produced in an HF alkylation process (67774-74-7)
Remark: Separate tests were conducted with LAB dissolved in acetone and LAB without solvent. In the first test, acetone-assisted concentrations of 0.05, 0.1, 0.2, 0.4, 0.8, 1.0, 1.2, and 1.4 mg/L were prepared. In the second test, a saturated LAB solution (0.040 mg/L) was tested as is and diluted to 0.030, 0.020, 0.010, and 0.005 mg/L. Results of the first test show that LAB is not toxic to Daphnia at the limit of solubility. In the second test the EC50 was 1.1 mg/L, which is much higher than the solubility concentration.
Source: Verge at al 1999.
Reliability: (1) valid without restriction
03-OCT-2001 (47)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: > .1
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: **GLP:** no data
Test substance: other TS: Phenyl-C10 (C10 LAB)
Remark: A distinction was made between immobilized and effected. No effects were observed up to 48 hours. The study was extended out to 144 hours and the EC50s were 0.083 at 96 hours, 0.035 at 120 hours, and 0.025 at 144 hours. The results show that the absence of toxicity can be related to the limited exposure period. If the exposure time is expanded up to 5 days, the EC50 values for waterborne exposures reach the solubility level. This hypothesis is clearly consistent with the assumption of non-polar narcosis as mode of action and toxicity related to the total body burden of LAB. Due to the low water solubility, prolonged waterborne exposures are required to reach the lethal body burden, as has been demonstrated for other poorly soluble hydrocarbons.
Source: Fernandez et al 2000.
Reliability: (1) valid without restriction
03-OCT-2001 (15)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Selenastrum capricornutum (Algae)
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: > 1000
Method: other: EPA 600/9-78-018 The Selenastrum capricornutum Printz algal assay
Year: 1978 **GLP:**
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Remark: Selenastrum capricornutum is not affected after 96 hours at nominal concentration (1000 mg/L) up to and exceeding the water solubility with a solvent carrier.
Source: Gledhill et al 1991.
Reliability: (1) valid without restriction
25-JUL-2001 (16)

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:**
EC50: > .1
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 **GLP:**
Test substance: other TS: LAB (67774-74-7) and individual homologues (phenyl C8, phenyl C10, phenyl C12, phenyl C14)
Remark: LAB concentrations tested were 0.025, 0.050, and 0.100 mg/L. No inhibition of growth was observed for LAB or any of the individual homologues.
Source: Moreno et al 2000.
Reliability: (1) valid without restriction
03-OCT-2001 (33)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type:
Species:
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species:
Endpoint:
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001
01

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species:

Endpoint:

Exposure period:

Unit:

Analytical monitoring:

Method:

Year:

GLP:

Test substance:

Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001**TERRESTRIAL ORGANISMS****4.6.1 Toxicity to Soil Dwelling Organisms**

Type:

Species:

Endpoint:

Exposure period:

Unit:

Method:

Year:

GLP:

Test substance:

Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-20
01**4.6.2 Toxicity to Terrestrial Plants**

Species:

Endpoint:

Expos. period:

Unit:

Method:

Year:

GLP:

Test substance:

Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001**4.6.3 Toxicity to other Non-Mamm. Terrestrial Species**

Species:

Endpoint:

Expos. period:

Unit:

Method:

Year:

GLP:

Test substance:

Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

4.7 Biological Effects Monitoring

Memo: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

4.8 Biotransformation and Kinetics

Type:
Remark: Not a High Production Volume Challenge Program endpoint.
03-OCT-2001

4.9 Additional Remarks

Memo: None
03-OCT-2001

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Sex: male/female
Number of Animals:
Vehicle: other: none
Value: > 5000 mg/kg bw
Method: other: OECD Guide-line 401: Rats were given a single oral administration by gavage.
Year: **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7). Average side chain length of 11.1 to 11.8.
Remark: No deaths were observed. Pilo-erection was observed shortly after dosing in all treated rats.
Source: Huntingdon Research Centre 1984.
Reliability: (2) valid with restrictions
Data as reported in LAB Risk Assessment, revised June 1997.
25-JUL-2001 (21)

Type: LD50
Species: rat
Sex: male/female
Number of Animals: 5
Vehicle:
Value: > 10000 mg/kg bw
Method: other: Undiluted test material was provided to three male and two female rats in a single oral dose.
Year: 1978 **GLP:** no data
Test substance: other TS: L-210H and L-210L (68608-80-0)
Remark: No signs of toxicity were observed with the exception of some weight loss on one to two days. Viscera were normal after 14 days. An earlier study by the same laboratory (1973) tested at a higher dose resulted in an LD50 > 15,800 mg/kg bw.
Source: Younger Laboratories 1978.
Reliability: (2) valid with restrictions
03-OCT-2001 (50)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time:
Value: > 1.82 mg/l
Method: other
Year: **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7). Average side chain length of 11.1 to 11.8.
Method: The substance was administered as an aerosol containing > 90% particles with diameter less than 10 microns.
Remark: No deaths were observed.
Source: Monsanto 1982.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision. Original report not reviewed.
25-JUL-2001 (31)

Type: LC50
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time:
Value: = 71 mg/l
Method: other
Year: **GLP:** no data
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Method: The substance was administered as an aerosol.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision. Original report not reviewed.
25-JUL-2001 (45)

Type: LC50
Species: rat
Sex: male
Number of Animals: 6
Vehicle: other: none
Exposure time: 6 hour(s)
Value: > .9 mg/l
Method:
Year: 1973 **GLP:** no data
Test substance: other TS: Benzene C6-12 alkyl derivs. (68608-80-0)
Method: A.T.S. Sprague-Dawley albino male rats were exposed in a 35 L inhalation chamber for 6 hrs at 27 degrees Celcius. The air flow rate was 4.0 L/min.
Remark: Four studies were performed with the same results. The concentrations of test substance in the different studies were 0.9, 0.55, 0.3, and 0.34 mg/L.

Result: No significant toxic signs were observed in any of the studies. Viscera appeared normal after 14 days.
Source: Younger Laboratories 1973; Younger Laboratories 1978.
Reliability: (2) valid with restrictions
03-OCT-2001 (49) (50)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rat
Sex: male/female
Number of Animals:
Vehicle: no data
Value: > 2000 mg/kg bw
Method: OECD Guide-line 402 "Acute dermal Toxicity"
Year: **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7). Average side chain length of 11.1 to 11.8.
Result: After a single dermal administration in rats, no deaths were observed, no signs of systemic toxicity were observed, and terminal autopsy findings were normal.
Source: Huntingdon Research Centre 1984.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.
25-JUL-2001 (20)

Type: LD50
Species: other: New Zealand Albino Rabbits
Sex: male/female
Number of Animals: 7
Vehicle: no data
Value: > 1260 mg/kg bw
Method: **GLP:** no data
Test substance: other TS: Benzene, C6-12-alkyl derivs. (68608-80-0) (L-210H)
Method: One male or female was exposed dermally to six doses (794, 1000, 1260, 2000, 3160, 5110 mg/kg) of undiluted test substance for 24 hours. The animals were observed for 14 days.
Result: All animals exposed to doses up to 1260 mg/kg survived. Mortality occurred for animals exposed to doses of 2000 mg/kg and higher. Weight loss was observed at two through six days in survivors. Animals in the higher concentrations experienced increasing weakness, collapse, and death. Gross autopsy of the decedents included lung and liver hyperemia, enlarged gallbladder, darkened kidneys, and gastrointestinal inflammation. Viscera appeared normal in the surviving animals.
Source: Younger Laboratories 1978.
Reliability: (2) valid with restrictions
03-OCT-2001 (50)

Type: LD50
Species: other: New Zealand Albino Rabbits
Sex: male/female
Number of Animals: 4
Vehicle: no data
Value: > 2000 mg/kg bw
Method: other: One male or one female was exposed dermally to four doses (1260, 2000, 3160, 5010 mg/kg) of undiluted test substance for 24 hours. The animals were observed for 14 days.
Year: **GLP:** no data
Test substance: other TS: Benzene, C6-12-alkyl derivs. (68608-80-0) (L-210L)
Result: All animals exposed to doses up to 2000 mg/kg survived while mortality occurred for animals exposed to the two highest doses. Weight loss was observed at two to four days in survivors. Animals in the higher concentrations experienced increasing weakness, collapse, and death. Gross autopsy of the decedents included lung and liver hyperemia, enlarged gallbladder, darkened kidneys, and gastrointestinal inflammation. Viscera appeared normal in the surviving animals.
Source: Younger Laboratories 1978.
Reliability: (2) valid with restrictions
25-JUL-2001 (50)

Type: LD50
Species: other: New Zealand Albino Rabbits
Sex: male/female
Number of Animals: 4
Vehicle: no data
Value: > 5010 mg/kg bw
Method: other: One male or one female rabbit was exposed to three doses (3160, 5010, 7940 mg/kg) of the undiluted test substance for 24 hours. The animals were observed for 14 days.
Year: **GLP:** no data
Test substance: other TS: Benzene, C6-12-alkyl derivs. (68608-80-0) (L210H + L210L)
Result: Animals exposed to 3160 and 5010 mg/kg survived. Female and male rabbits exposed to the 7940 mg/kg dose died on days 2 and 10, respectively. Signs of intoxication included reduced appetite and activity (days four to seven in survivors), increasing weakness, collapse, and death. Gross autopsy of the decedents revealed hemorrhagic lungs, mottled and discolored liver, enlarged gallbladder, and gastrointestinal inflammation. Viscera in the survivors appeared normal.
Source: Younger Laboratories 1973.
Reliability: (2) valid with restrictions
03-OCT-2001 (48) (49)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.v.
Value: = 3493 mg/kg bw
Method:
Year: GLP: no data
Test substance: other TS: Pentadecane (C15 normal paraffin) (629-62-9)
Source: Louis 1996.
Reliability: (4) not assignable
25-JUL-2001 (28)

5.2 Corrosiveness and Irritation**5.2.1 Skin Irritation**

Species:
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result:
EC classificat.:
Method:
Year: GLP:
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
01-NOV-2001

5.2.2 Eye Irritation

Species:
Concentration:
Dose:
Exposure Time:
Comment:
Number of
Animals:
Result:
EC classificat.:
Method:
Year: GLP:
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
01-NOV-2001

5.3 Sensitization

Type:
Species:
Number of
Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
01-NOV-2001

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: inhalation
Exposure period: 70 day(s) (14 week period)
Frequency of
treatment: 6 hours per day/5 days per week
Post. obs.
period:
Doses: 0, 102, 298, or 580 mg LAB per cubic meter of air in 10m3
inhalation chambers
Control Group: yes, concurrent no treatment
NOAEL: = 102 ppm
Method: other: EPA/TSCA.
Year: GLP: yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Method: 15 male and 15 female rats were exposed per group.
Remark: Skin and mucous membrane irritation and respiratory problems
were evident at the mid- and high exposure concentrations.
Body weight gains were also depressed at these levels. While
liver weights and serum levels of hepatic enzymes were
elevated in females from the high concentrations, there were
no gross or histopathological changes.
Source: Monsanto 1986.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997
revision.
25-JUL-2001 (32)

5. Toxicity

date: 08-NOV-2001
Substance ID: Atops

Species: rat **Sex:**
Strain: no data
Route of admin.: oral feed
Exposure period: 4 weeks
Frequency of treatment: daily in diet
Post. obs. period:
Doses: various concentrations up to 20000 ppm (2%)
Control Group:
LOAEL: = 125 mg/kg bw
Method: other: EPA/TSCA
Year: **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Remark: Reduction in body weight and food consumption were observed at all exposure levels. No gross pathological changes were noted. Histopathology was not carried out. The lowest dose tested was 2500 ppm, which corresponds to 125 mg/kg bw.
Source: Monsanto.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.

25-JUL-2001

(30)

Species: mouse **Sex:**
Strain:
Route of admin.:
Exposure period: 20 weeks
Frequency of treatment:
Post. obs. period:
Doses:
Control Group:
LOAEL: = 9600 mg/kg
Method:
Year: **GLP:**
Test substance: other TS: Tetradecane (629-59-4)
Remark: Patty's reports this result as "the lowest toxic dose (TDLo) of tetradecane for mice is 9600 mg/kg for 20 weeks." No further information is provided and Patty's lists only an incorrect citation. Therefore, then reliability of this value cannot be determined.
Source: Sandmeyer 1981.
Reliability: (4) not assignable

08-NOV-2001

(39)

5.5 Genetic Toxicity 'in Vitro'

Type: Bacterial reverse mutation assay
System of testing: Salmonella typhimurium TA 1535, TA 100, TA 1537, and TA 98
Concentration: 0, 100, 1000, 4000, 8000, and 10000 ug/plate
Metabolic activation: with and without
Result: negative
Method: Directive 84/449/EEC, B.14 "Other effects - Mutagenicity (Salmonella typhimurium - reverse mutation assay)"
Year: 1984 **GLP:** no data
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Source: Bronzetti et al 1991.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.

01-NOV-2001

(4)

Type: Mammalian cell gene mutation assay
System of testing: Chinese Hamster Ovary (CHO) cells
Concentration: 100 to 2000 micrograms/mL
Metabolic activation: with and without
Result: negative
Method: other: EPA/TSCA
Year: **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Remark: V79/HGPRT and Saccharomices cerevisiae genetic toxicity studies conducted on LAB by other authors also showed negative results.
Result: There were no statistically significant increases in mutation frequencies for the substance compared to the negative control. Cytotoxicity was significant at and above 1250 micrograms/mL with and without metabolic activation.
Source: Robinson and Nair 1992.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997 revision.

25-JUL-2001

(35)

Type: Bacterial reverse mutation assay
System of testing: Salmonella typhimurium TA 1535, TA 100, TA 1537, and TA 98
Concentration: .03, 12, 60, 300, 1000, 3000 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: EPA/TSCA
Year: **GLP:** yes
Test substance: other TS: Benzene C10-13 alkyl derivs. (LAB) (67774-74-7)
Remark: The highest concentration produced evidence of either toxicity or insolubility.
Source: Robinson and Nair 1992.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997

02-NOV-2001 revision.

(35)

5.6 Genetic Toxicity 'in Vivo'

Type: other: Bone marrow chromosome aberration assay
Species: rat **Sex:** male/female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: single treatment
Doses: 1200, 4000, and 12700 mg/kg bw
Result: negative
Method: other: EPA/TSCA - Bone marrow chromosome aberration
Year: 1992 **GLP:** yes
Test substance: other TS: LAB undiluted or dissolved in corn oil (67774-74-7)
Result: A significant mean body weight loss was found in the groups treated with the highest dose. No statistically significant increases in chromosomal aberration or gaps were observed in the treated groups in any of the sampling times. Both mean chromosome numbers and mean mitotic indices were similar in test and vehicle control groups.
Source: Robinson and Nair 1992.
Reliability: (2) valid with restrictions
Data reported in LAB Risk Assessment Report, June 1997
revision.

25-JUL-2001

(35)

5.7 Carcinogenicity

Species: **Sex:**
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Post. obs. period:
Doses:
Result:
Control Group:
Method:
Year: **GLP:**
Test substance:
Remark: Not a High Production Volume Challenge Program endpoint.
01-NOV-2001

5.8 Toxicity to Reproduction

Type: Two generation study
Species: rat **Sex:**
Strain: other: CD (Charles River Breeding Laboratories)
Route of admin.: gavage
Exposure Period: 35 weeks
Frequency of treatment: single daily dose
Premating Exposure Period
 male: 10 weeks
 female: 10 weeks
Duration of test: 35 weeks
Doses: 0, 5, 50, and 500 mg/kg/d
Control Group:
NOAEL Parental: = 50 mg/kg bw
NOAEL F1 Offspr.: = 50 mg/kg bw
Method: other
 Year: **GLP:** no data
Test substance: other TS: linear alkylbenzene in corn oil (67774-74-7)
Method: Four groups of 30 male and 30 female were given the test substance by gavage once daily for about 10 weeks before mating. Once mated (as evidence by a copulatory or sperm in the vaginal smear), females were housed separately for the remainder of gestation. Females were dosed during mating, gestation and lactation for a total of 127 days of treatment. After weaning, 30 males and 30 females of the F1 generation were dosed for an 11-week premating period. Dosing of F1 females continued through mating, gestation, and lactation. All of the resulting F2 pups were euthanized on day 13 of gestation.
Remark: All adults and pups received a gross post-mortem examination. Histopathology studies were conducted on reproductive tissues, tissues with gross lesions, and the pituitary gland taken from each adult in the control and high dose groups.
Result: There was evidence of toxicity in adults and offspring at the 500 mg/kg/day dose level, with the most consistent effects being depressed weight gains in adults, smaller litters, and fewer live pups; decreased pup survival and lower pup survival at some intervals. At 50 mg/kg/day, only a reduction in F1 of pup weight gain on day 7 was observed, but this effect had returned to normal at days 14 and 21. This temporary reduction in pup weight occurred in one generation, and this was not consistent across generations. Based on the significant effects at 500 mg/kg/day and the non consistent effects at the lower dose, the NOAEL for reproductive toxicity is 50 mg/kg/day for both parental and neonatal animals.
Source: Robinson and Nair 1992.
Reliability: (2) valid with restrictions
03-OCT-2001 (35)

5.9 Developmental Toxicity/Teratogenicity

Species: rat **Sex:** female
Strain: other: CD (Charles River Breeding Laboratories)
Route of admin.: gavage
Exposure period: days 6-15 of gestation
Frequency of treatment: single daily dose
Duration of test: 20 days
Doses: 125, 500, and 2000 mg/kg bw/day
Control Group:
NOAEL Maternalt.: = 125 mg/kg bw
Method: other
Year: **GLP:** yes
Test substance: other TS: Alkylate 215 (68648-87-3) as a surrogate for LAB (67774-74-7)
Method: Groups of 24 mated rats were given the test substance in corn oil on days 6-15 of gestation. Rats were observed twice daily and the body weights recorded on gestation days 0, 6, 10, 12, 15, and 20. Fetuses were delivered by caesarean section on gestation day 20 and the numbers of live, dead, and researched fetuses, total implantations, and corpora lutea were recorded. Fetuses and surviving mated females received post mortem examinations.
Remark: The substance should not be considered as a developmental toxicant since an increased incidence of ossification variations and delayed ossification only at dose levels including maternal toxicity cannot be considered as specific effects on prenatal development.
Result: Depressed maternal food consumption and weight gains were observed at 500 mg/kg/day and 2000 during treatment, but significantly increased in the post treatment period. No treatment-related increases in soft tissue malformations and variations were observed in either the maternal or fetal generations. Some skeletal malformations (wavy ribs) and ossification variations were observed in the highest doses.
Source: Robinson and Schroeder 1992.
Reliability: (1) valid without restriction
03-OCT-2001 (36)

5.10 Other Relevant Information

Type:
Remark: None
03-OCT-2001

5.11 Experience with Human Exposure

Memo: None
03-OCT-2001

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7.1 Risk Assessment

Memo: Refer to LAB Alkylate Top Assessment Plan
01-NOV-2001